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Marcelo Pereyra, Nicolas Dobigeon, Hadj Batatia, Jean-Yves Tournet. Computing the Cramer-Rao bound of Markov random field parameters: Application to the Ising and the Potts models. IEEE Signal Processing Letters, Institute of Electrical and Electronics Engineers, 2014, vol. 21, pp. 47-50. <10.1109/LSP.2013.2290329>. <hal-00915825>

HAL Id: hal-00915825

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To link to this article : doi:10.1109/LSP.2013.2290329
URL : <http://dx.doi.org/10.1109/LSP.2013.2290329>

To cite this version : Pereyra, Marcelo and Dobigeon, Nicolas and Batatia, Hadj and Tourneret, Jean-Yves Computing the Cramer-Rao bound of Markov random field parameters: Application to the Ising and the Potts models. (2014) IEEE Signal Processing Letters, vol. 21 (n° 1). pp. 47-50. ISSN 1070-9908

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Computing the Cramer–Rao Bound of Markov Random Field Parameters: Application to the Ising and the Potts Models

Marcelo Pereyra, Nicolas Dobigeon, Hadj Batatia, and Jean-Yves Tournet

Abstract—This letter considers the problem of computing the Cramer–Rao bound for the parameters of a Markov random field. Computation of the exact bound is not feasible for most fields of interest because their likelihoods are intractable and have intractable derivatives. We show here how it is possible to formulate the computation of the bound as a statistical inference problem that can be solve approximately, but with arbitrarily high accuracy, by using a Monte Carlo method. The proposed methodology is successfully applied on the Ising and the Potts models.

Index Terms—Cramer–Rao bound, intractable distributions, Markov random fields, Monte Carlo algorithms.

I. INTRODUCTION

THE estimation of parameters involved in intractable statistical models (i.e., with intractable likelihoods) is a difficult problem that has received significant attention in the recent computational statistics and signal processing literature [1], [2], [3], [4]. Particularly, estimating the parameters of a Markov random field (MRF) is an active research topic in image processing [5], [6], [7], [8], [9]. Several new unbiased estimators have been recently derived, mainly based on efficient Monte Carlo (MC) methods [1], [2], [9], [10].

This letter addresses the problem of computing the Cramer–Rao bound (CRB) [11] for estimators of MRF parameters. Knowing the CRB of a statistical model is of great importance for both theoretical and practical reasons. From a theoretical point of view, the CRB establishes a lower limit on how much information a set of observations carries about unknown parameters. Specifically, it defines the minimum variance for any unbiased estimator of these parameters. From

a practical perspective, the CRB is used as a means to characterize the performance of unbiased estimators in terms of mean square error (i.e., estimation variance). Unfortunately, the CRB for most MRF models is difficult to compute because their likelihoods are intractable [12, Chap. 7].

This letter addresses this difficulty by formulating the computation of the CRB as a statistical inference problem that can be solved using MC methods [13]. Precisely, we propose to express the CRB in terms of expectations that can be efficiently estimated by MC integration [13, Chap. 3]. The proposed CRB estimation method is demonstrated on specific MRF models that have been widely used in the image processing community, namely the Potts and Ising models. The remainder of the letter is organized as follows: Section II defines the class of statistical models considered in this work and proposes an original method to estimate their CRB based on a MC algorithm. The application of the proposed methodology to the Ising and Potts models is presented in Section III. Conclusions are finally reported in Section IV.

II. COMPUTING THE FISHER INFORMATION MATRIX $\mathcal{I}(\theta)$

Let $\theta = (\theta_1, \dots, \theta_M)^T$ be an unknown parameter vector and $z = (z_1, z_2, \dots, z_N)^T$ an observation vector whose elements take their values in a set Ω . This paper considers the case where θ and z are related by the following generic distribution

$$f_{\theta}(z) \triangleq \frac{1}{C(\theta)} \exp [\theta^T \Phi(z)] \quad (1)$$

where $\Phi(z) : \Omega^N \rightarrow \mathbb{R}^M$ is a sufficient statistic and $C(\theta)$ is the normalizing constant given by

$$C(\theta) = \int_{\Omega^N} \exp [\theta^T \Phi(z)] dz. \quad (2)$$

where integration is performed in the Lebesgue sense with respect to an appropriate measure on Ω^N . Note that the model (1) defines an important subclass of the exponential family. It comprises several standard distributions, such as Gaussian, Laplace or gamma distributions, as well as multivariate distributions frequently used in signal and image processing applications, such as Markov random fields [12]. In this latter case, the normalizing constant, also known as partition function, is generally intractable owing to the inherent difficulty of evaluating integrals over Ω^N when N is large [12].

The Cramer–Rao bound of θ establishes a lower bound on the covariance matrix of any unbiased estimator $\hat{\theta}$ of θ [11]. Because the existence of the bound requires that $f_{\theta}(z)$ verifies

The work of M. Pereyra was supported by the SuStaIn program, EPSRC Grant EP/D063485/1 from the Department of Mathematics, University of Bristol, and by a postdoctoral fellowship from French Ministry of Defence. This work was developed as part of the DynBrain project, supported by the 6th STIC-AmSud program. The associate editor coordinating the review of this manuscript and approving it for publication was Prof. Gustavo Camp-Valls.

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some weak regularity conditions, we will assume that $C(\theta)$ is continuously differentiable (i.e., $C(\theta) \in C^1$). Then the CRB is equal to the inverse of the Fisher information matrix (FIM) of θ [11], i.e.,

$$\text{cov}(\hat{\theta}) \geq \text{CRB}(\theta) = [\mathcal{I}(\theta)]^{-1} \quad (3)$$

where the inequality (3) means that the matrix $\text{cov}(\hat{\theta}) - [\mathcal{I}(\theta)]^{-1}$ is positive semidefinite and where $\mathcal{I}(\theta)$ is an $M \times M$ positive semidefinite symmetric matrix whose element (i, j) is given by [11]

$$\mathcal{I}_{i,j}(\theta) \triangleq \mathbb{E}_f \left[\frac{\partial}{\partial \theta_i} \log[f_\theta(\mathbf{z})] \frac{\partial}{\partial \theta_j} \log[f_\theta(\mathbf{z})] \right] \quad (4)$$

where \mathbb{E}_f denotes the expectation operator with respect to $f_\theta(\mathbf{z})$. By applying the definition (4) to (1) we obtain that

$$\begin{aligned} \mathcal{I}_{i,j}(\theta) = \mathbb{E}_f \left[\left(\Phi_i(\mathbf{z}) - \frac{\partial}{\partial \theta_i} \log C(\theta) \right) \right. \\ \left. \times \left(\Phi_j(\mathbf{z}) - \frac{\partial}{\partial \theta_j} \log C(\theta) \right) \right] \end{aligned} \quad (5)$$

where $\Phi_i(\mathbf{z}) : \Omega^N \rightarrow \mathbb{R}$ is the i th component of the vector field $\Phi(\mathbf{z}) = [\Phi_1(\mathbf{z}), \dots, \Phi_M(\mathbf{z})]^T$. Unfortunately, evaluating (5) for MRF models is rarely possible because of the intractability of the derivatives $\frac{\partial}{\partial \theta_i} \log C(\theta)$. Note that difficulty cannot be addressed by numerical differentiation because $\log C(\theta)$ is itself intractable.

This letter proposes to exploit a property of the exponential family to replace the intractable derivatives in $\mathcal{I}(\theta)$ by expectations that can be efficiently approximated using MC integration [13, Chap. 3]. Precisely, we use the following property that relates the derivatives $\frac{\partial}{\partial \theta_i} \log C(\theta)$ to the expectations of Φ [14, p. 118]

$$\begin{aligned} \frac{\partial}{\partial \theta_i} \log[C(\theta)] &= \frac{1}{C(\theta)} \int_{\Omega^N} \Phi_i(\mathbf{z}) \exp[\theta^T \Phi(\mathbf{z})] d\mathbf{z} \\ &= \mathbb{E}_f [\Phi_i(\mathbf{z})]. \end{aligned} \quad (6)$$

Again, integration is performed in the Lebesgue sense with respect to an appropriate measure on Ω^N . By substituting property (6) in equation (5) we obtain the matrix

$$\mathcal{I}(\theta) = \text{cov}[\Phi(\mathbf{z})] \quad (7)$$

whose elements are

$$\mathcal{I}_{i,j}(\theta) = \mathbb{E}_f [\Phi_i(\mathbf{z})\Phi_j(\mathbf{z})] - \mathbb{E}_f [\Phi_i(\mathbf{z})] \mathbb{E}_f [\Phi_j(\mathbf{z})]. \quad (8)$$

The property (6) has been used previously to derive the statistical moments of Φ from the derivatives of $C(\theta)$ in cases where $C(\theta)$ is known and can be differentiated analytically [15, p. 116] as well as to study the physical properties of lattice systems [16, Chap. 31]. However, to the best of our knowledge this is the first time that this property is used in a statistical inference context to compute a CRB.

Expression (8) differs from (5) by the fact that derivatives are replaced by expectations of Φ w.r.t. $f_\theta(\mathbf{z})$. From a computational perspective this alternative expression is fundamentally better than (5) because the expectations, in spite of being intractable, can be efficiently approximated with arbitrarily high

accuracy by MC integration [13, Chap. 3]. Note that MC approximations are particularly well suited for high-dimensional models given that their accuracy depends exclusively on the number of MC samples used and not on the dimension of the model.

Lastly, approximating $\mathcal{I}(\theta)$ by MC integration requires simulating samples distributed according to $f_\theta(\mathbf{z})$. In this letter, this is achieved by using a Gibbs sampler that admits $f_\theta(\mathbf{z})$ as unique stationary distribution [13]. This sampler belongs to the class of Markov chain Monte Carlo (MCMC) algorithms, which are interesting for MRFs because they not require to know $C(\theta)$. The output of this algorithm is a Markov chain of N_{MC} samples $\{\mathbf{z}^{(t)}\}_{t=1}^{N_{\text{MC}}}$ that can be used to approximate $\mathcal{I}(\theta)$ through the sample covariance matrix

$$\hat{\mathcal{I}}(\theta) = \sum_{t=1}^{N_{\text{MC}}} \frac{(\mathbf{u}^{(t)} - \bar{\mathbf{u}})(\mathbf{u}^{(t)} - \bar{\mathbf{u}})^T}{N_{\text{MC}} - 1}, \quad \mathbf{u}^{(t)} = \Phi(\mathbf{z}^{(t)}) \quad (9)$$

with $\bar{\mathbf{u}} = \sum_{t=1}^{N_{\text{MC}}} \mathbf{u}^{(t)} / N_{\text{MC}}$. The ergodicity of the Gibbs sampler guarantees that as the number of samples increases $\hat{\mathcal{I}}(\theta)$ converges to $\mathcal{I}(\theta)$ (for details about MCMC algorithms and their practical application please see [13], [17]). Moreover, note that $\hat{\mathcal{I}}(\theta)$ is semipositive definite by construction and it is invertible whenever N_{MC} is large enough such that $\{\mathbf{u}^{(t)}\}_{t=1}^{N_{\text{MC}}}$ spans \mathbb{R}^M . In practice this condition is satisfied almost surely if N_{MC} is large enough to produce a stable estimate of $\mathcal{I}(\theta)$. Finally, note that (9) is valid regardless of the specific MCMC method used to simulate from $f_\theta(\mathbf{z})$. For simplicity this letter considers that samples are generated using a Gibbs sampler, which provides a general solution that it is easy to apply to any given MRF [12]. However, the Gibbs sampler is not always the most efficient method to simulate from a specific MRF (e.g., the Ising and Potts models are more efficiently sampled with a Swendsen-Wang algorithm [18]). More details about the proposed Monte Carlo scheme are provided in a separate technical report [19].

III. APPLICATION TO THE ISING AND POTTS MARKOV RANDOM FIELDS

A. Ising and Potts Models

This section applies the proposed methodology to the computation of the CRB of two important intractable models, namely the homogeneous Ising and Potts MRF. For completeness these models are recalled below.

Let $\mathbf{z} = (z_1, z_2, \dots, z_N)$ be a discrete random vector whose elements take their values in the finite set $\Omega_K = \{1, \dots, K\}$. The Ising and the Potts MRF are defined by the following probability mass function

$$f_\theta(\mathbf{z}) \triangleq \frac{1}{C(\theta)} \exp[\theta \Phi(\mathbf{z})] \quad (10)$$

with

$$\Phi(\mathbf{z}) = \sum_{n=1}^N \sum_{n' \in \mathcal{V}(n)} \delta(z_n - z_{n'}) \quad (11)$$

where $\mathcal{V}(n)$ is the index set of the neighbors associated with the n th element, $\delta(\cdot)$ is the Kronecker function and $\theta \in \mathbb{R}^+$ is the

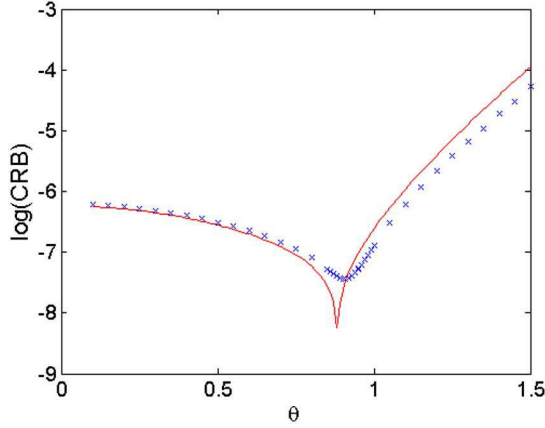


Fig. 1. Cramer–Rao bound for an Ising (MRF) defined on a toroidal graph. True CRB (solid red), estimates obtained by MC integration (blue crosses).

granularity coefficient or *inverse temperature* parameter. The Gibbs distribution (10) corresponds to the Ising MRF when $K = 2$, and to the Potts MRF for $K \geq 3$. In our experiments $\mathcal{V}(n)$ will be considered to be a bidimensional first-order (i.e., 4-pixel) neighborhood structure. However, the proposed method is valid for any correct neighborhood structure (see [12] for more details). Finally, note that despite their simplicity these models are extensively used in modern image segmentation and/or classification applications (see [20], [21] and references therein) and that the estimation of the granularity parameter θ is still an active research topic [9].

B. Validation With Ground Truth

To validate the proposed MC method under controlled conditions (i.e., for a known CRB), the proposed methodology has been first applied to an Ising model defined on a *toroidal* graph (i.e., with cyclic boundary conditions) of size $N = 32 \times 32$. Unlike most MRF models, this particular MRF has a known normalizing constant and FIM [8].

Fig. 1 compares the estimates obtained for different values of θ with the true CRB [8]. These estimates have been computed from Markov chains of 1 000 000 samples generated with a Gibbs sampler. More details about this experiment are provided in a separate technical report [19].

We observe in Fig. 1 that the estimates obtained with the proposed method are in good agreement with the true values of the CRB. We also observe that the error introduced by using a Monte Carlo approximation varies slightly with the value of θ and is larger at approximately $\theta = 0.9$, coinciding with the phase-transition temperature of the Ising MRF ($\theta_c = \log(1 + \sqrt{2}) \approx 0.88$). These variations with θ are due to the fact that the mixing properties of the Gibbs sampler deteriorate at temperatures close to θ_c due to long range dependencies between the elements of \mathbf{z} [13, p. 339]. As a result the Markov chains associated with different values of θ have different effective samples sizes [13, p. 499] (i.e., different numbers of equivalent independent samples) and produce estimates with different accuracies. Indeed, the effective sample size, measured from the chain’s autocorrelation function, is 870 000 samples for $\theta = 0.1$, it decreases progressively to 20 000

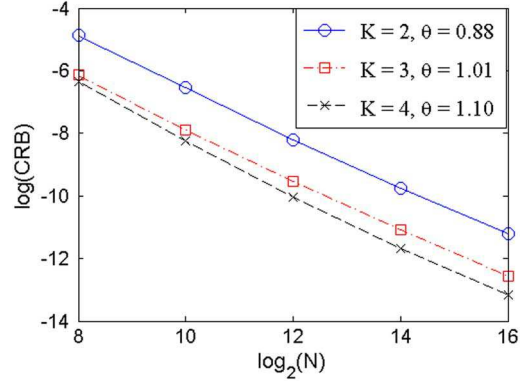


Fig. 2. Cramer–Rao bound for an Ising ($K = 2$) and two Potts MRF ($K = 3$ and $K = 4$) close to phase-transition and for different field sizes N . Results are displayed in *log-log* scales.

samples for $\theta = 0.9$ and then increases to 235 000 samples for $\theta = 1.5$.

C. Asymptotic Study of the CRB

The second set of experiments shows the evolution of the CRB with respect to the size of observation vector \mathbf{z} (i.e., the number of field components N). The CRB has been computed for the following 5 field sizes $N = (2^8, 2^{10}, 2^{12}, 2^{14}, 2^{16})$, corresponding to bidimensional MRFs of size 16×16 , 32×32 , 64×64 , 128×128 and 256×256 . Experiments have been performed using an Ising MRF, a 3-state and a 4-state Potts MRF (i.e., $K = 2$, $K = 3$ and $K = 4$ respectively) defined on a regular lattice (not a toroid). CRB estimates have been computed from Markov chains of 2500 000 samples. Finally, for each model, the parameter θ was set close to the critical phase-transition value, i.e., $\theta_c = \log(1 + \sqrt{K})$ to introduce a strong dependency between the components of the MRF. Fig. 2 shows the resulting CRBs versus the size of the MRF N in logarithmic scales.

We observe that for all models the logarithm of the CRB decreases almost linearly with the logarithm of the number of field components. This result shows that the strong dependency between the field components does not modify significantly the linear behavior that is generally observed for models defined by statistically independent components. We also observe that the CRB decreases with the number of states K , indicating that an accurate estimation of θ for the Ising model is more difficult than for a Potts MRF.

D. Evaluation of State-of-the Art Estimators of θ

The third set of experiments compares the CRB to the empirical variance of three state-of-the art estimation methods, the *auxiliary variable* [1], *exchange* [2] and *ABC* [9] algorithms. As explained previously, the CRB is often used as a means to measure the performance of unbiased estimators in terms of mean square error. In this letter, the three algorithms studied in [1], [2], [9] have been used to compute an approximate maximum-likelihood (ML) estimation of θ for the 3-state Potts MRF (additional results with an Ising MRF are provided in a separate technical report [19]).

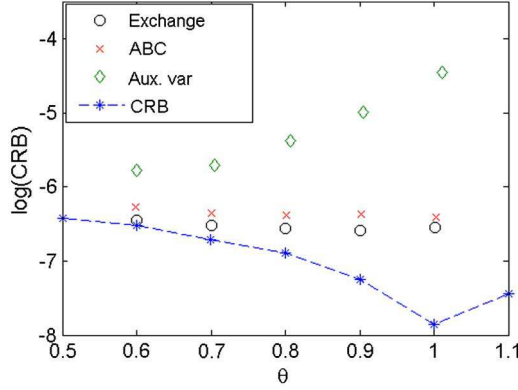


Fig. 3. Cramer–Rao bounds for a 3-state Potts models of size 32×32 . Results are displayed in logarithmic scale.

Experiments were conducted as follows. First $N_{ML} = 2500$ synthetic observation vectors $\mathbf{z}^{(i)} \sim f_{\theta}(\mathbf{z})$, $i = 1, \dots, N_{ML}$ were generated using an appropriate Gibbs sampler. Then, for each observation $\mathbf{z}^{(i)}$, three ML estimates $\hat{\theta}_{EXCH}^{(i)}$, $\hat{\theta}_{ABC}^{(i)}$ and $\hat{\theta}_{AUX}^{(i)}$ were computed using the three estimation methods mentioned above. Finally, the variance of each estimator was approximated by computing the sample variance, e.g., $\text{Var}(\hat{\theta}_{ABC}) = (N_{ML} - 1)^{-1} \sum_{i=1}^{N_{ML}} (\hat{\theta}_{ABC}^{(i)} - \bar{\theta}_{ABC})^2$ with $\bar{\theta}_{ABC} = N_{ML}^{-1} \sum_{i=1}^{N_{ML}} \hat{\theta}_{ABC}^{(i)}$. More details about this experiment are provided in a separate technical report [19].

Fig. 3 compares the CRB estimated with our method for the 3-state Potts MRF with the variance of the ML estimates obtained with the state-of-the art algorithms. These values have been computed for $\theta < \theta_c$ which is the range of interest for this model (for $\theta > \theta_c$ all the field components have almost surely the same color). We observe the good performance of the ML estimators based on the exchange [2] and the ABC [9] for small values of θ (i.e., $\theta < 0.8$). However, their performance decreases progressively for $\theta > 0.8$, a behavior that is explained by the fact that the estimators use a Gibbs sampler to approximate the intractable likelihood. As explained previously, the mixing properties of this sampler deteriorate as θ increases towards the critical value θ_c . This results in a degradation of the approximation of the likelihood and in a larger ML variance. Moreover, one can also see that the estimator based on the auxiliary variable method [1] has a larger variance than the others for all values of θ . This result is in accordance with the experiments reported in [2], [9].

IV. CONCLUSION

This letter studied the problem of computing the CRB for the parameters of Markov random fields. For these distributions the CRB depends on the derivatives of the normalizing constant or partition function $C(\theta)$, which is generally intractable. This difficulty was addressed by exploiting an interesting property of the exponential family that relates the derivatives of the normalizing constant $C(\theta)$ to expectations of the MRF potential. Based on this, it was proposed to estimate the Fisher information matrix of the MRF (and therefore the CRB) using a Monte Carlo method. The proposed approach was successfully applied to the Ising and the Potts models, which are frequently used

in signal processing applications. The resulting bounds have been used, in turn, to assess the statistical efficiency of three state-of-the-art estimation methods that are interesting for image processing applications. An extension of the proposed method to hidden MRFs is currently under investigation. Perspectives for future work include the derivation of Bayesian bounds for intractable models whose unknown parameters are assigned prior distributions.

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